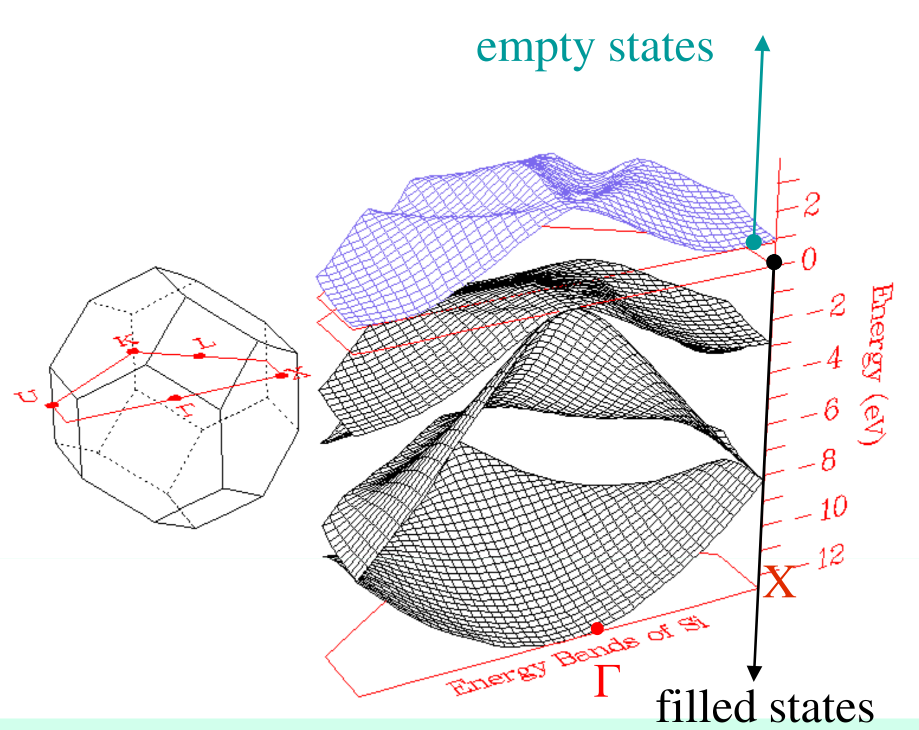
PHYSICAL MECHANISMS OF INTERFACE-MEDIATED INTERVALLEY COUPLING IN SILICON

André L. Saraiva – UFRJ – Brazil

Si Qubit Workshop – Berkeley 2009

Saraiva *et al.* PRB **80**, 081305R (2009)

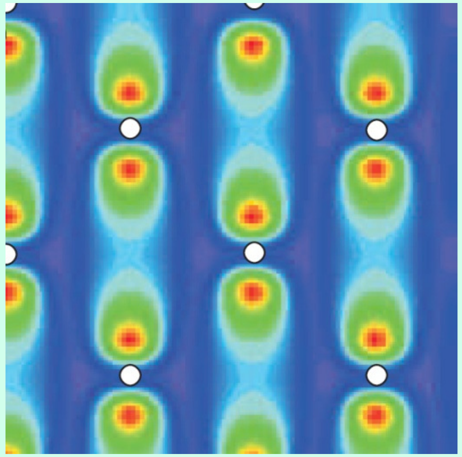
Bulk Si Electronic Structure



<u>Bloch States</u>

$$\phi_{k_\mu}(\vec{r}) = e^{i\vec{k}_\mu \cdot \vec{r}} \; u_{\vec{k}_\mu}(\vec{r})$$

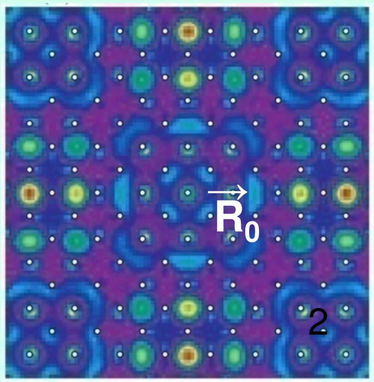
$$\left|\phi_{k_\mu}(\vec{r})\right|^2 \rightarrow$$



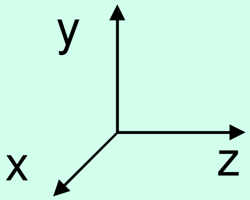
Koiller *et al* [PRB(2004)]

Any superposition of degenerate Bloch states
is also an eigenstate (not in Bloch's form).
Example:

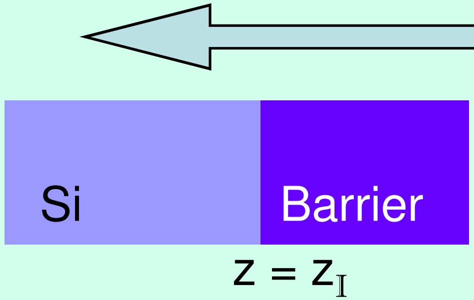
$$\phi(\vec{r}) = \frac{1}{\sqrt{6}} \sum_{\mu=1,6} \phi_{\vec{k}_\mu}(\vec{r} - \vec{R}_0) \;\Rightarrow\; |\phi(\vec{r})|^2 \;\mapsto$$



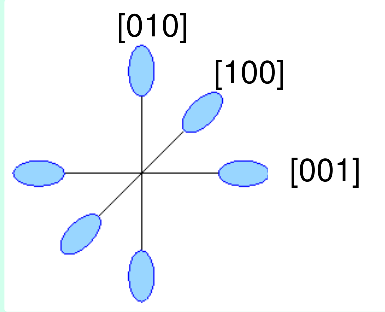
Lifting the Degeneracy



$\vec{F}$



$$k_0 \approx 0.85\frac{2\pi}{a_0}$$



$$H = H_0 + H'$$

$$E_{\pm k_x} = E_{\pm k_y}$$

$$E_{\pm k_x} = E_{\pm k_y} = E_{\pm k_z}$$

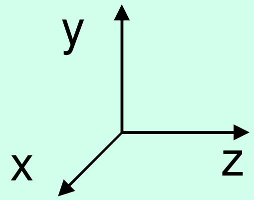
$$E_{\pm k_z}$$

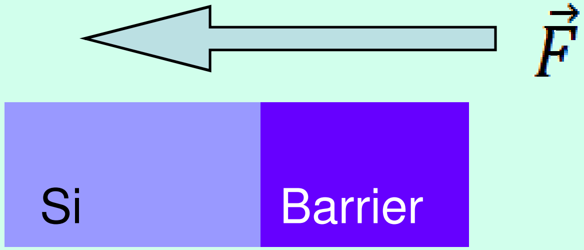
$$E_0 \propto \left(\frac{F^2}{m_z}\right)^{\frac{1}{3}} \xrightarrow{yields} \Delta_{xz}$$

$$\approx 20 - 30 \text{ meV}$$

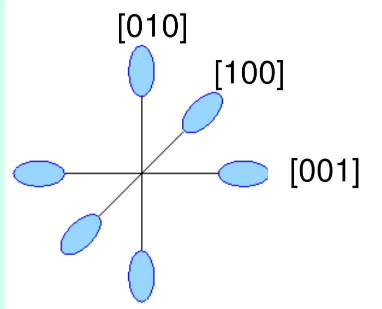
$$\varphi(\vec{r}) = a_+\phi_{+z} + a_-\phi_{-z}$$

Lifting the Degeneracy

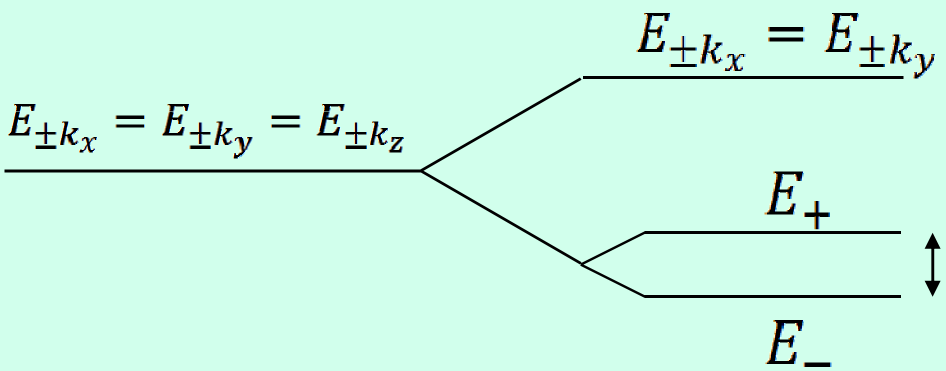




$$k_0 \approx 0.85 \frac{2\pi}{a_0}$$



$$H = H_0 + H'$$



$2|V_{VO}|$

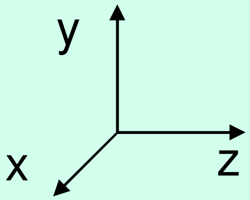
$\approx 20 - 30\ \mathrm{meV}$

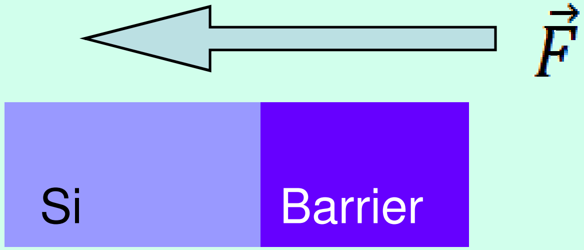
$\approx 0.01 - 1\ \mathrm{meV}$

$$H = \begin{pmatrix} E_0 & V_{VO} \\ V_{VO}^* & E_0 \end{pmatrix}$$

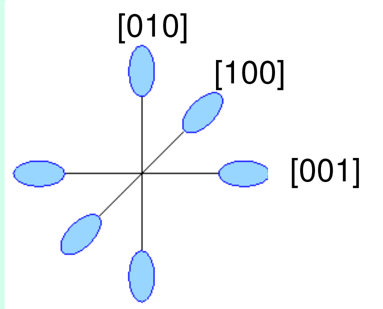
$$\boxed{V_{VO} = \langle \phi_- | H' | \phi_+ \rangle}$$

Lifting the Degeneracy

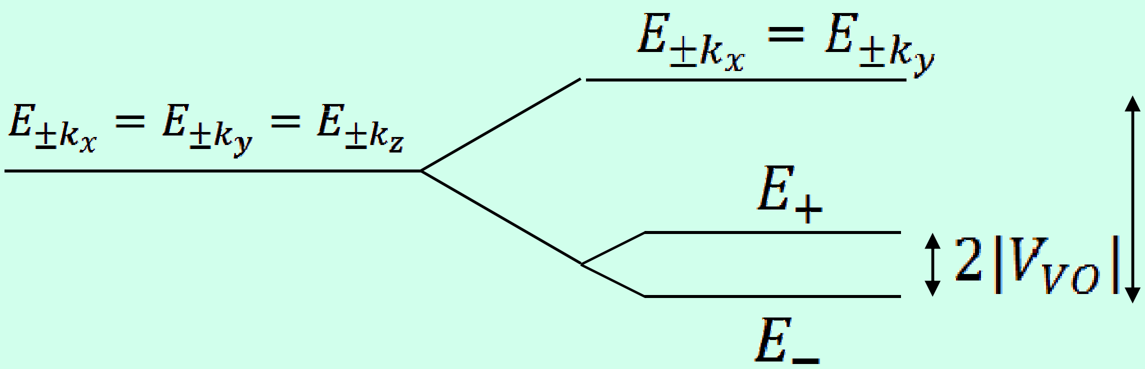




$$k_0 \approx 0.85\frac{2\pi}{a_0}$$



$$H = H_0 + H'$$



$$E_0 \propto \left(\frac{F^2}{m_z}\right)^{\frac{1}{3}} \xrightarrow{yields} \Delta_{xz}$$

$$\approx 20 - 30 \text{ meV}$$

PRL **96,** 236801 (2006) PHYSICAL REVIEW LETTERS week ending 16 JUNE 2006

Valley Polarization in Si(100) at Zero Magnetic Field

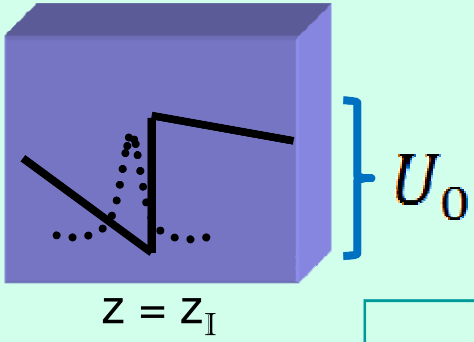
$2|V_{VO}| \rightarrow 23$ meV

K. Takashina,[1] Y. Ono,[1] A. Fujiwara,[1] Y. Takahashi,[1,*] and Y. Hirayama[1,2]
[1]*NTT Basic Research Laboratories, NTT Corporation, Atsugi-shi, Kanagawa 243-0198, Japan*
[2]*SORST JST, Kawaguchi, Saitama 331-0012, Japan*

(Received 28 April 2005; published 12 June 2006)

Effective Mass Theory – Step Model

$$H' = U(z) - eFz \Rightarrow$$



$$U(z) = U_0\Theta(z - z_I)$$

Finite Differences Method
(Fine Description of Evanescent Tail)

• <u>Single Valley Eff. Mass Equation</u>

$$\left[-\frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2} + U(z) - eFz\right]\psi(z) = E_0\psi(z)$$

$$\phi_\pm(\vec{r}) = \psi(z)e^{\pm i\vec{k}_0\cdot\vec{r}}\left[\sum_{\vec{G}} c_\pm(\vec{G})e^{i\vec{G}\cdot\vec{r}}\right]$$

$$V_{VO} = \langle\phi_-|H'|\phi_+\rangle$$

Plane Waves Expansion Coefficients
Kohn Orbitals- DFT

Effective Mass Theory – Step Model

$z_I = 0$

$$V_{VO} = \sum_{\vec{G},\vec{G}'} c_+^*(\vec{G})\, c_-^*(\vec{G}')\ \delta(G_x - G_x{}')\ \delta(G_y - G_y{}') \times I(G_z, G_z')$$

$$I(G_z,G_z') = \int_{-\infty}^{\infty} |\Psi(z)|^2\, e^{iQz}\, [U_0\Theta(z)]\ dz - \int_{-\infty}^{\infty} |\Psi(z)|^2\, e^{iQz}\, [eFz]\ dz$$

$$= \int_{-\infty}^{\infty} \frac{i\, e^{iQz}}{Q} |\Psi(z)|^2 U_0 \delta(z)\, dz + \int_0^{\infty} \frac{i\, e^{iQz}}{Q} \frac{d}{dz} |\Psi(z)|^2 U_0\, dz + I_F$$

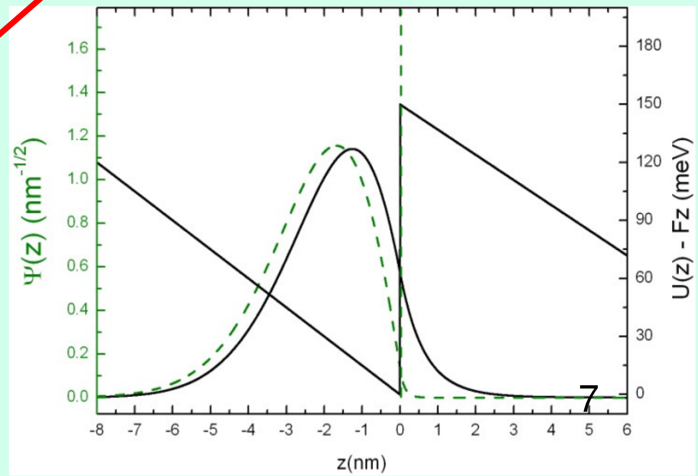
$$= i\frac{U_0}{Q}|\Psi(0)|^2 + i\frac{U_0}{Q}\int_0^{\infty} \frac{d}{dz}|\Psi(z)|^2\, e^{iQz}\ dz + I_F$$

$$Q \stackrel{\text{def}}{=} G_z - G_z' - 2k_0$$

Σ Σ Σ

$$V_{VO} = V_\delta + V_T + V_F$$

~ 0

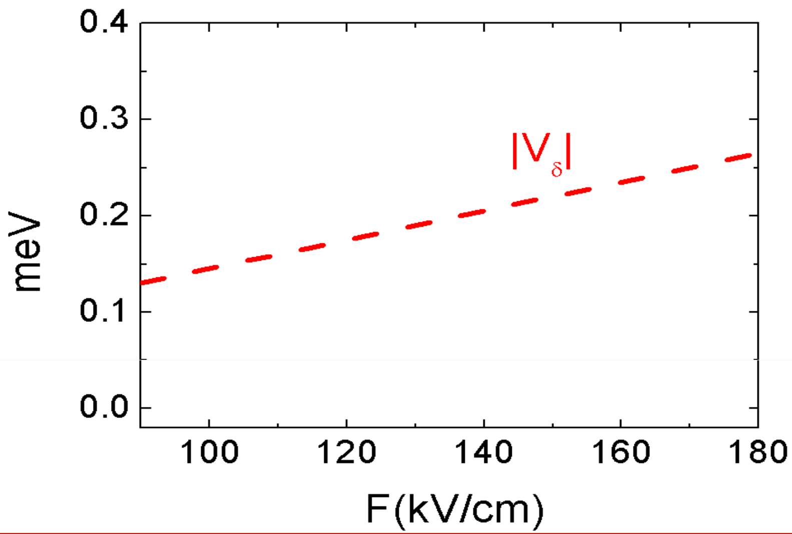


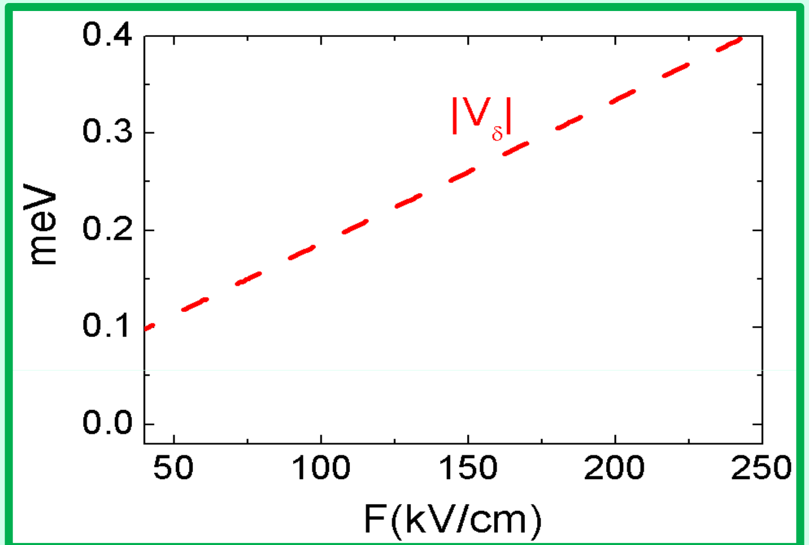
Step Model Results

$$V_\delta = U_0 |\Psi(0)|^2 \sum c_- c_+^* \delta_x \delta_y \frac{i}{Q}$$

U_0 = 150 meV ~ SiGe

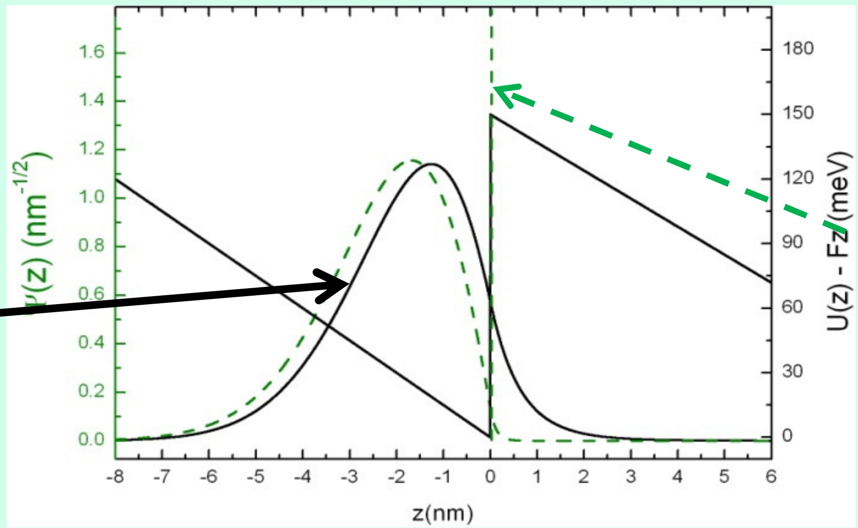
U_0 = 3 eV ~ SiO_2





Small U_0
Vs
Large $|\Psi(0)|^2$

Large U_0
Vs
Small $|\Psi(0)|^2$



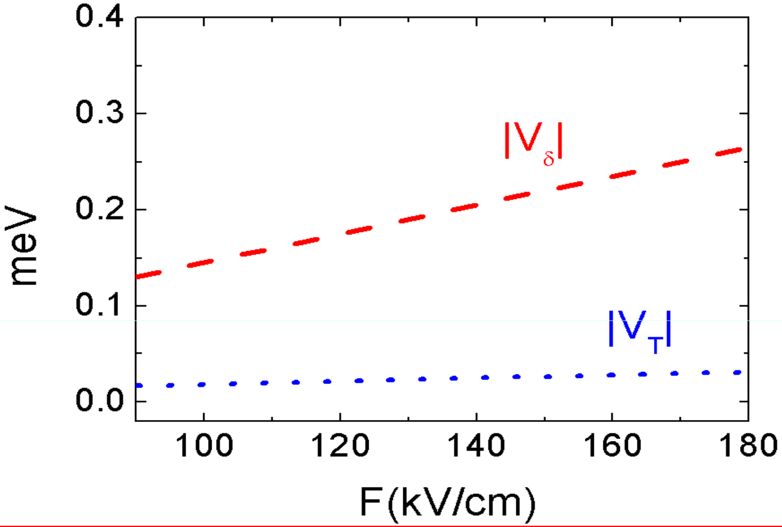
SiGe

SiO_2

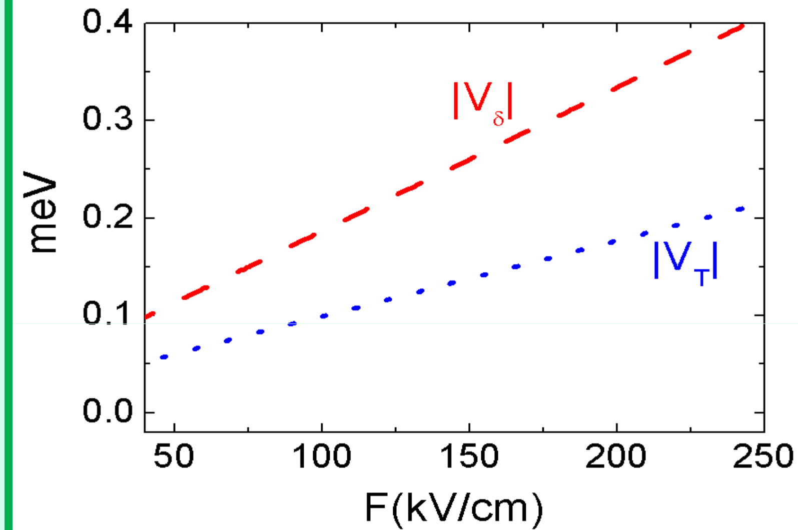
Step Model Results

$$V_T = \sum c_- c_+^* \delta_x \delta_y \int_0^\infty \frac{i\, e^{iQz}}{Q} \frac{d}{dz} |\Psi(z)|^2 U_0\, dz$$

U_0 = 150 meV ~ SiGe



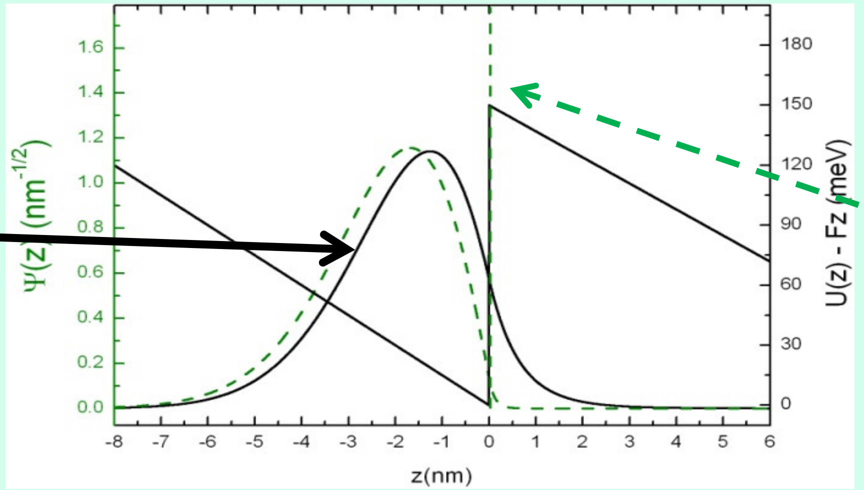
U_0 = 3 eV ~ SiO_2



Evanescent Tail
<u>much larger than</u>
Wavelength

Evanescent Tail
<u>comparable to</u>
Wavelength

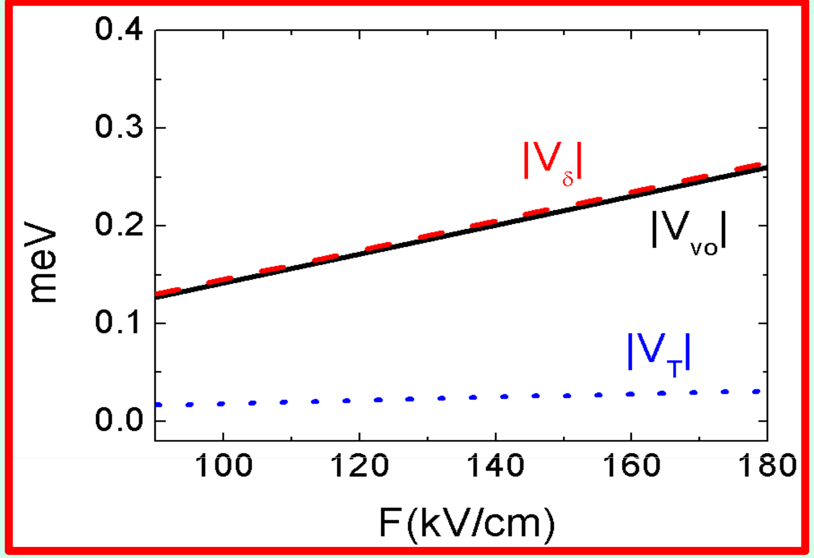
SiGe



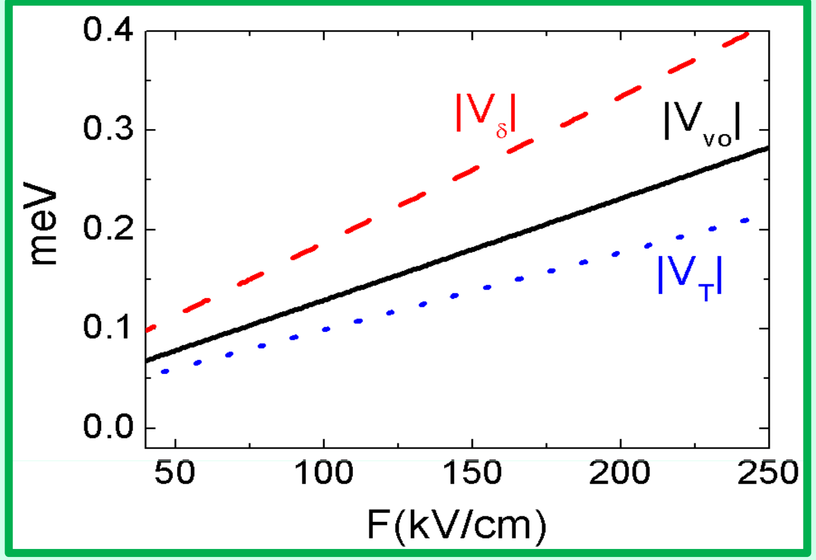
SiO_2

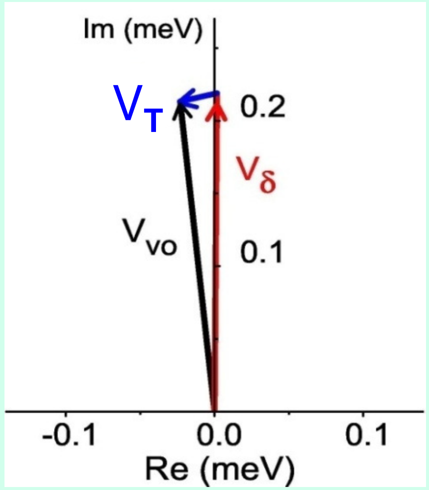
Step Model Results

U_0 = 150 meV ~ SiGe



U_0 = 3 eV ~ SiO_2



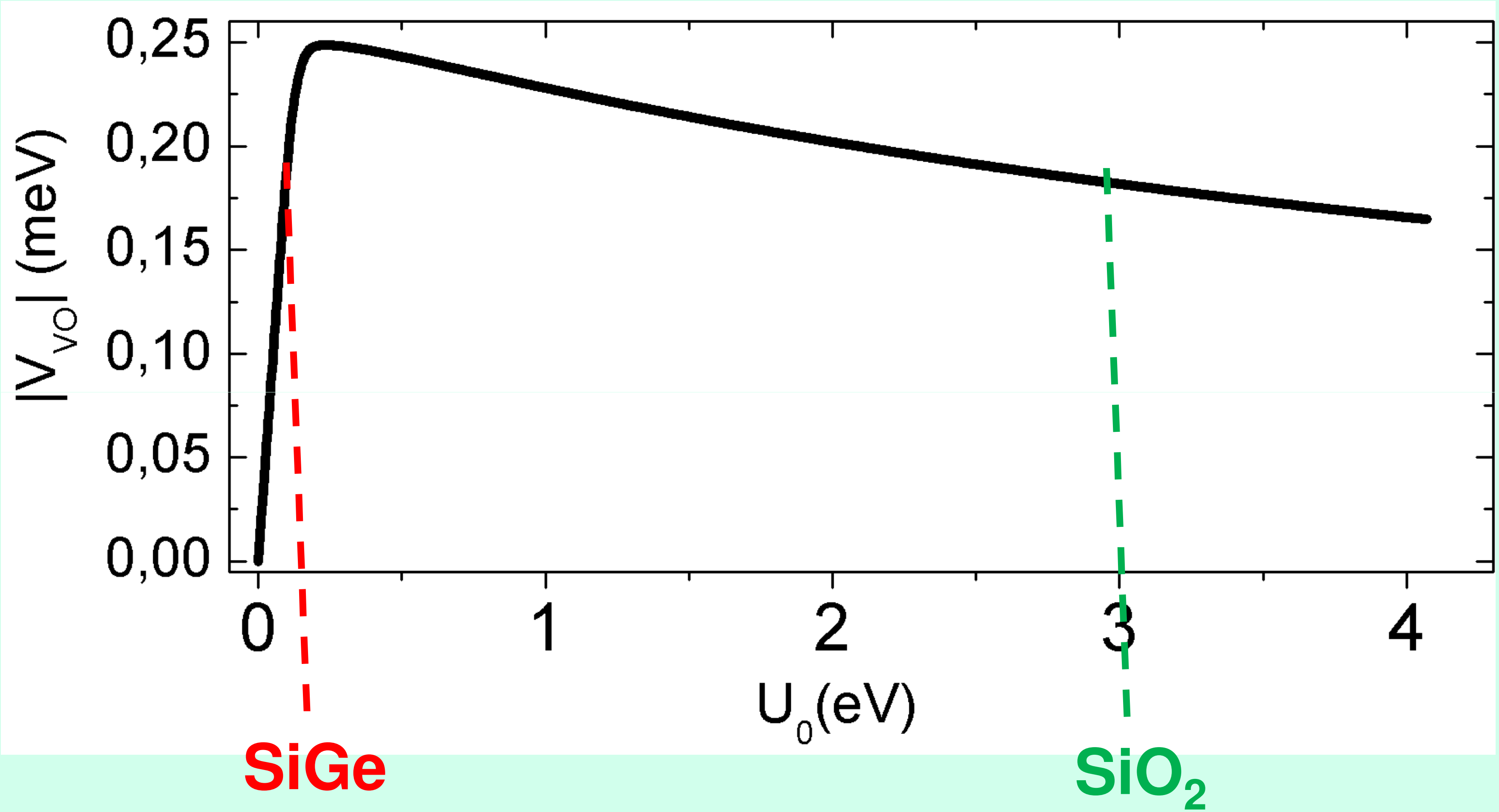


$$V_{VO} = V_\delta + V_T + V_F$$

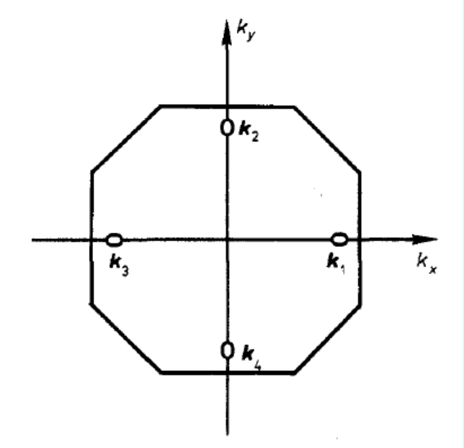
$$|V_{VO}| \approx 10 \text{ meV}$$

$$F \approx 10\,000 \text{ kV/cm!}$$

Role of the Barrier Material



Relevance of Umklapp Processes



R. Resta,
J. Phys. C (1977)

$$V_\delta = \nu\, |\Psi(0)|^2$$

$$\phi_\pm(\vec{r}) = \psi(z) e^{\pm i\vec{k}_0\cdot\vec{r}} \left[\sum_{\vec{G}} c_\pm(\vec{G})\, e^{i\vec{G}\cdot\vec{r}}\right]$$

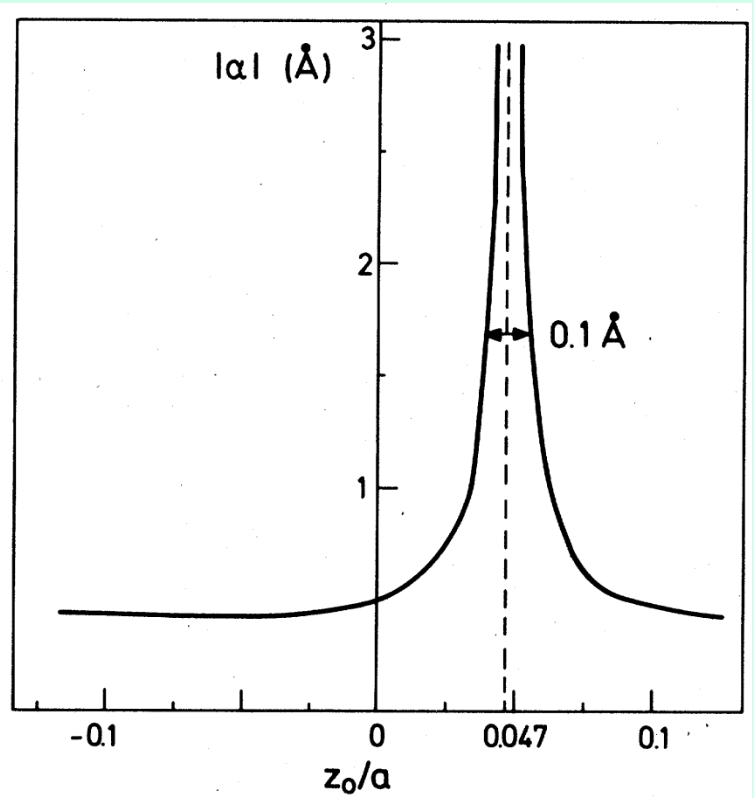
Taking only G=G'=0

$$\nu \approx 5.1 \times 10^{-11}\, U_0\ (\mathrm{eV\,.\,m})$$

Convergence on G
(up to second nearest neighbors from Γ in the BCC RL)

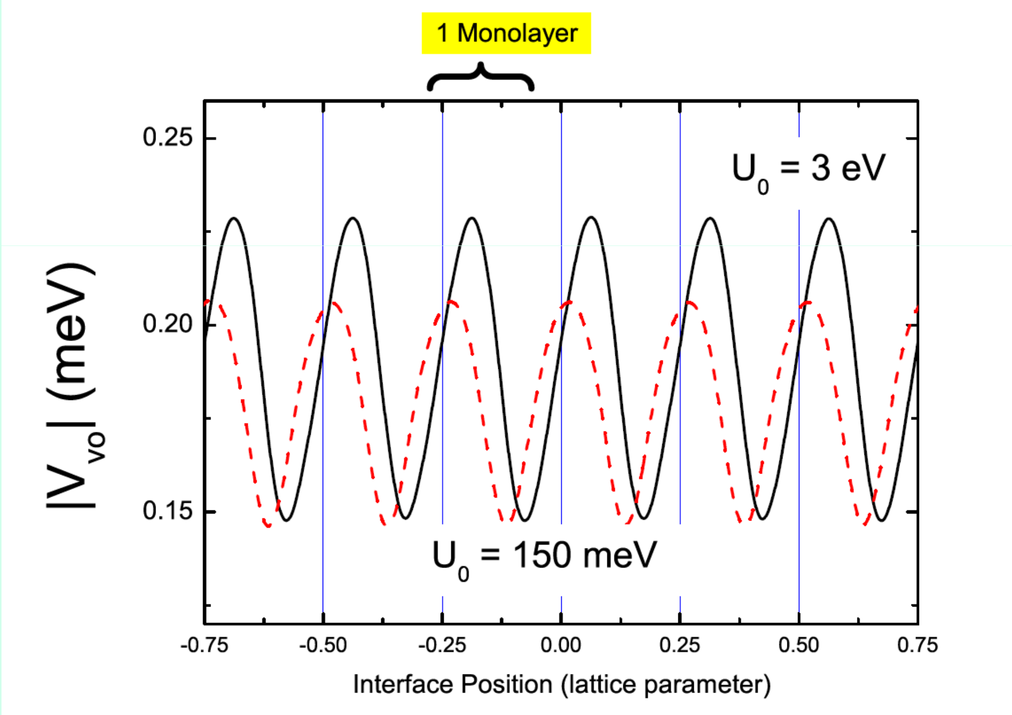
$$\nu \approx 1.6 \times 10^{-11}\, U_0\ (\mathrm{eV\,.\,m})$$

Interface Position



← 1 monolayer →

$$H = H_0 + U_0\Theta(z - z_I) - eFz$$



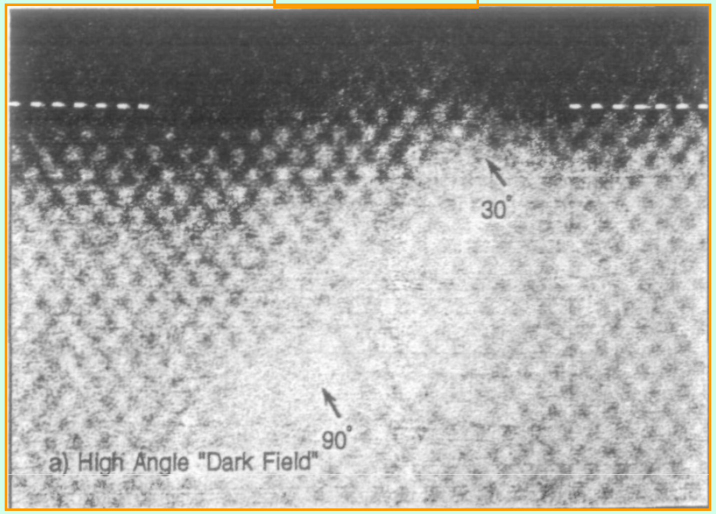
Scattering Length
L. Sham & M Nakayama,
PRB(1979)

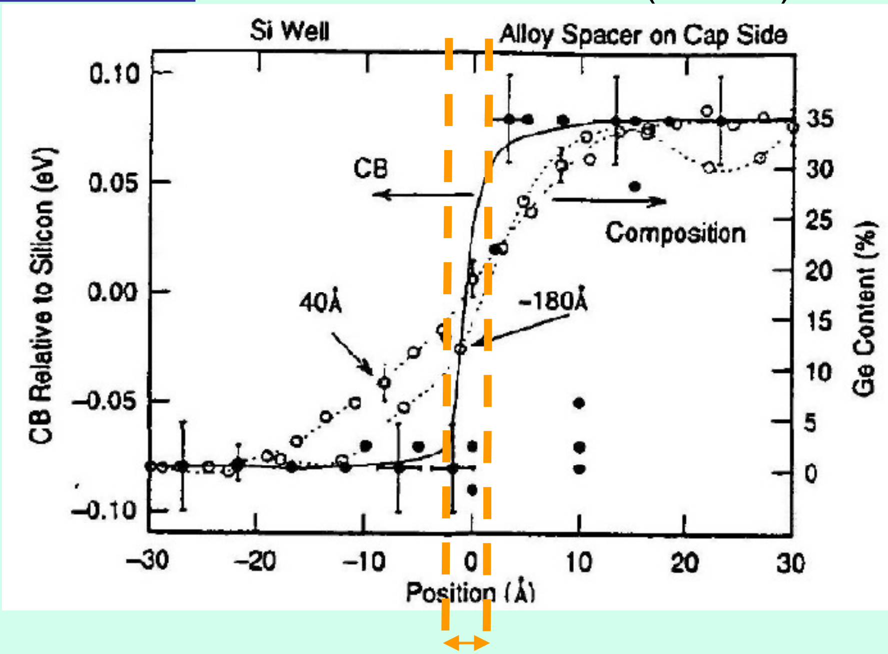
(Present Work)

Real Samples

(EELS)

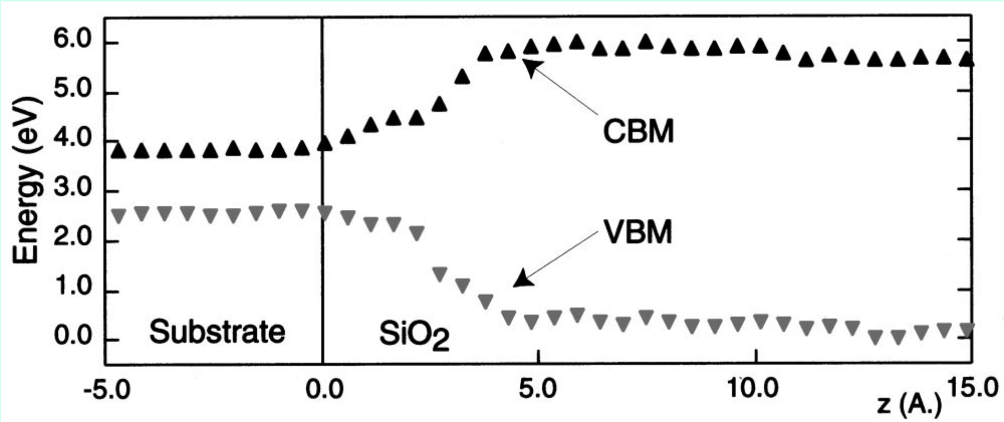
Si/SiGe





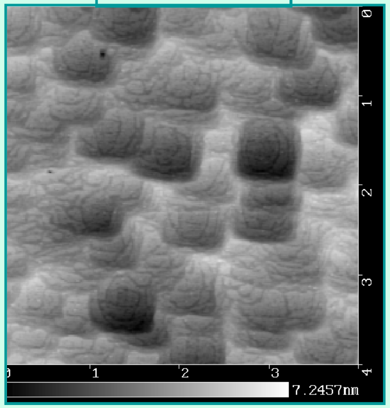
Batson [J. Elec. Micr.(2000)]

$\approx 1 - 2$ ML



Yamasaki *et al* [PRB(2004)]

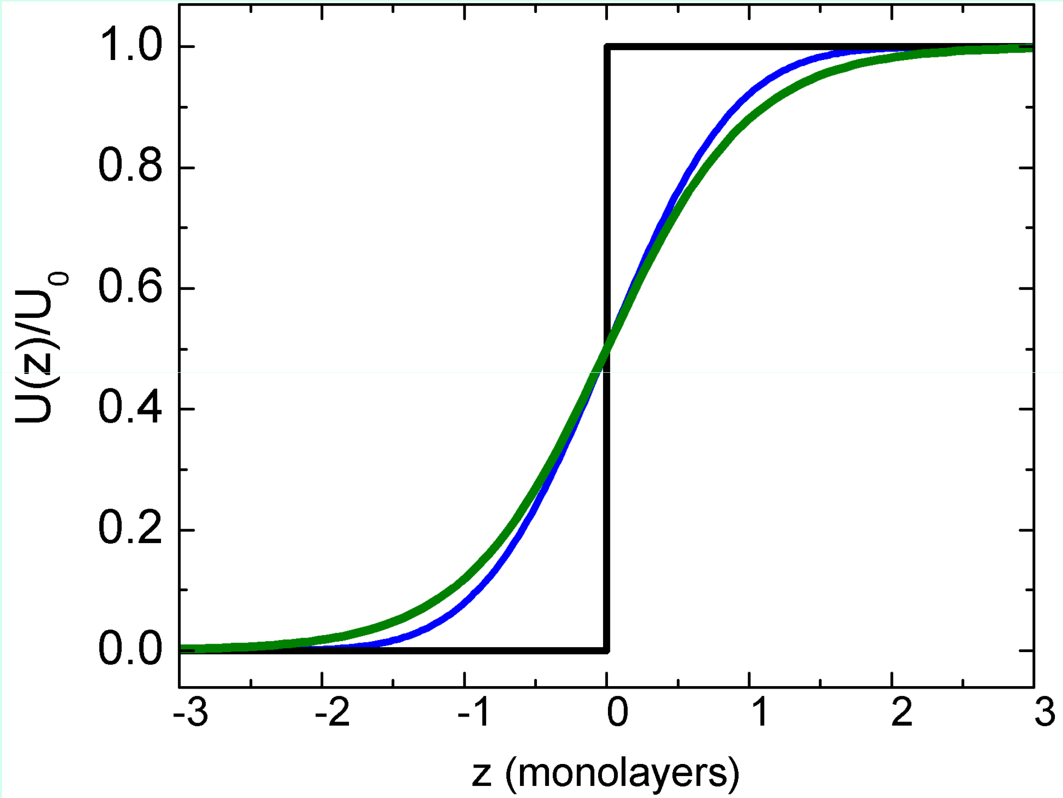
Si/SiO_2



Finite Width Models

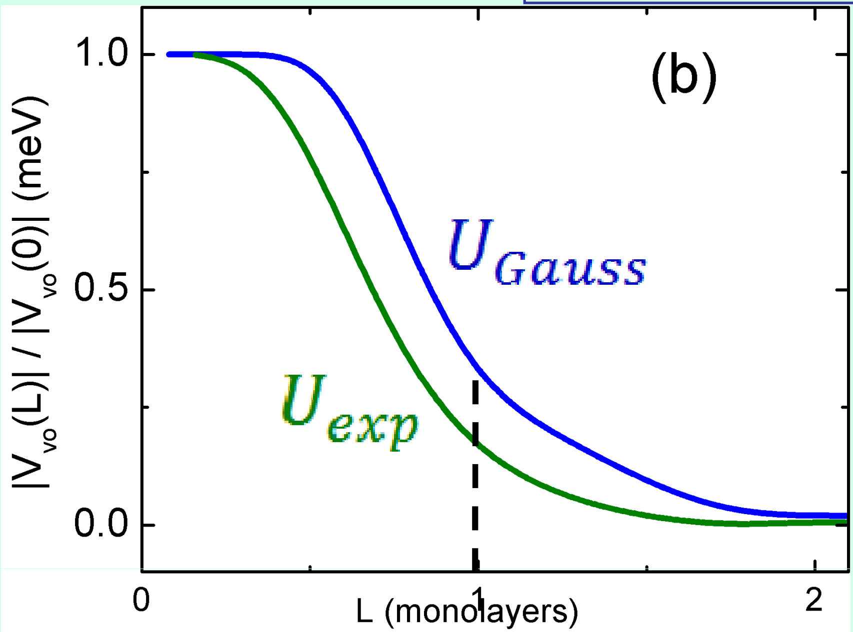
$$U_{exp} = \frac{U_0}{2}\left[\tanh\left(\frac{z}{L}\right) + 1\right]$$

$$U_{Gauss} = \frac{U_0}{2}\, erfc\left(-\frac{z}{L}\right)$$



RMS width of U_{exp} is 8% larger than RMS width of U_{Gauss}

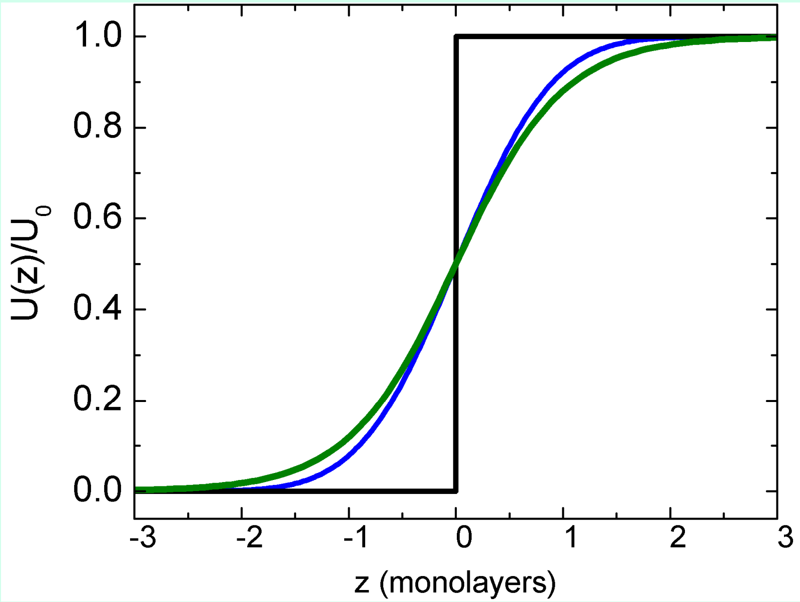
Results for Finite Width

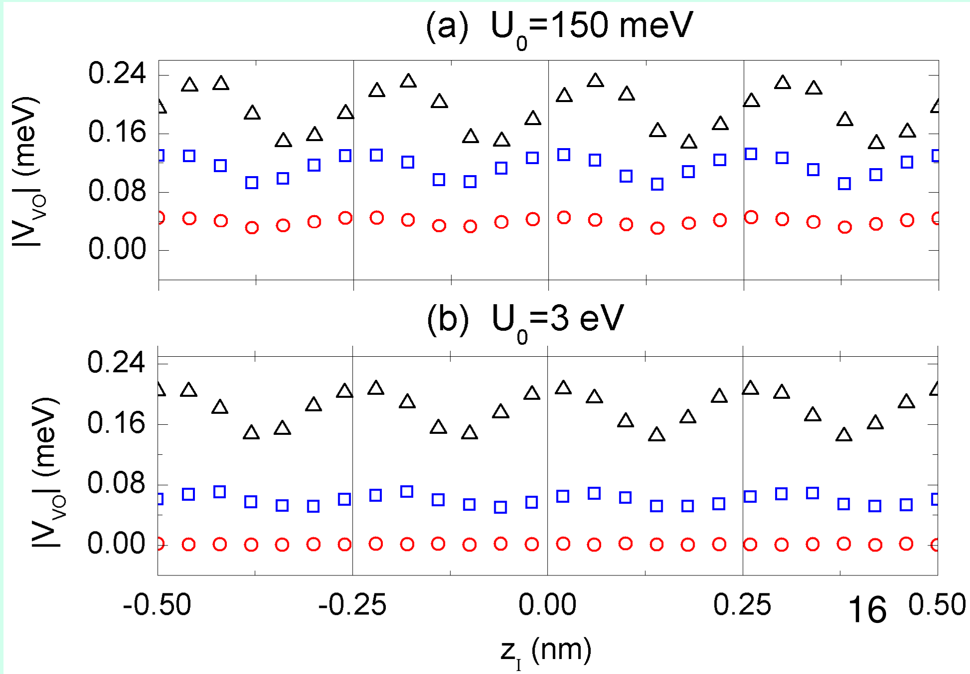


RMS width of U_{exp} is 8% larger than RMS width of U_{Gauss}

V_{VO} of U_{Gauss} is almost twice the V_{VO} of U_{exp}

L= 1 ML





Conclusions

• We identified nanofabrication parameters that might enhance interface-induced intervalley coupling;

• High quality heterostructures($L \longrightarrow 0$) are indeed more suitable for QC; no sign of intervalley coupling as large as 10 meV;

• V_{VO} could be further enhanced by some band structure engineering (design of suitable U_0);

•Effective Mass theory gives consistent description for the intervalley coupling, free of fitting parameters;

• The unphysical oscillations of V_{VO} with the interface position are artifacts of the effective mass theory in combination with atomistic Bloch Functions;

André L. Saraiva – UFRJ – also@if.ufrj.br

Maria J. Calderón – CSIC / Madrid
Xuedong Hu – Buffalo
Sankar Das Sarma – Maryland
Belita Koiller - UFRJ

Saraiva *et al.* PRB **80**, 081305R (2009)

Supported by Brazilian agencies: CNPq, FUJB,
Millennium Institute on Nanotechnology-MCT, and FAPERJ.

M.J.C. acknowledges funding from Ministerio de Ciencia e Innovación Spain through the Ramón y Cajal Program and through Grant No. MAT2006-03741.

X.H. and S.D.S. thank financial support by NSA and LPS through USARO and by NSF.